ANSWER 33 OF 37 CAPLY COPYRIGHT 2003 ACS on STN L3 1971:462924 CAPLUS Ionization constants of heterocyclic substances. IX. Protonation of AN DN aminopyridines and aminopyrimidinones ΤI John Curtin Sch. Med. Res., Aust. Natl. Univ., Canberra, Australia ΑU Journal of the Chemical Society [Section] B: Physical Orga CS SO (7), 1425-32CODEN: JCSPAC; ISSN: 0045-6470 Journal DTEnglish LΑ 33614-05-0 33630-96-5 IT RL: PRP (Properties) (ionization and uv spectrum of, in aq. soln.) 2(1H)-Pyridone, 5-amino-1-methyl-, conjugate monoacid (8CI) (CA INDEX RN CN

NAME)

● H<sup>+</sup>

RN 33630-96-5 CAPLUS CN 2(1H)-Pyridinone, 5-amino-1-methyl- (9CI) (CA INDEX NAME)

IT 33615-92-8P 33631-18-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

Patel

<11/9/2003>

10018688.11

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RN 33615-92-8 CAPLUS

CN 2(1H)-Pyridone, 5-amino-1-methyl-, hexachloroplatinate(2-) (2:1) (8CI) (CA INDEX NAME)

CM 1

CRN 33630-96-5 CMF C6 H8 N2 O

CM 2

CRN 16941-12-1 CMF C16 Pt . 2 H CCI CCS

●2 H+

RN 33631-18-4 CAPLUS

CN 2(1H)-Pyridone, 5-amino-1-methyl-, monopicrate (8CI) (CA INDEX NAME)

CM 1

CRN 33630-96-5

CMF C6 H8 N2 O

L3 ANSWER 26 OF 70 CAPLUS COPYRIGHT 2003 ACS on STN

AN 1994:95745 CAPLUS

DN 120:95745

TI Method of determining viability of tissue with adenosine/adenosine agonist and Al adenosine receptor antagonist

IN Mcafee, Donald A.; Belardinelli, Luiz

PA Whitby Research Inc., USA

SO U.S., 8 pp. CODEN: USXXAM

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ΡI	US 5117830	A	19920602	US 1990-610544	19901108
	US 5256398	Α	19931026	US 1992-828115	19920130
				US 1990-610544	19901108

## IT 131713-84-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and reaction of, in adenine deriv. prepn. for tissue viability detn.)

RN 131713-84-3 CAPLUS

CN Cyclopentanecarboxamide, N-[4-chloro-6-(methylamino)-5-pyrimidinyl]- (9CI) (CA INDEX NAME)

GΙ

Patel

<11/9/2003>

10018688.10

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ΑB A method and compn. is disclosed for detg. the viability of tissue in a region of an organism having a vascular circulatory system that supplies blood to the region; the method includes: (1) dilating the above vascular circulation system by introducing adenosine or an adenosine agonist into the vascular circulation system to increase the blood flow into the region; (2) introducing a blood flow marking medium into the region; (3) alleviating the non-dilating effects of adenosine or the adenosine agonist by introducing an Al adenosine receptor antagonist into the vascular circulatory system; and (4) detg. the amt. of marking medium in the region. The compns. of the invention include I [R1 = H, R2; R2 = endo-2-norbornyl, cyclopentyl; R3 = H, halo, amine, carboxy, C1-10 alkyl, etc.; R4 = benzyl, Ph, (O-substituted) C1-4 alkyl (e.g. ethers, alcs.); R5 = H, OH, sulfonate, halo, C1-6 (cyclo)alkoxy]. The method and compn. of the invention are useful in thallium-201 scintigraphy, and decrease side effects through alleviating the Al effects of adenosine as an Al antagonist while maintaining the A2 vasodilation activity of adenosine. Prepn. of selected I is included, and various I were assayed in Al and A2

ANSWER 49 OF 70 CAPLUS COPYRIGHT 2003 ACS on STN Ľ3 ΑN

DN

Reactions of benzenediazonium ions with adenine and its derivatives TI ΑU

D-+-1

CS Dep. Chem., Univ. Chicago, Chicago, IL, 60637, USA Journal of Organic Chemistry (1981), 46(11), 2203-7 so

CODEN: JOCEAH: ISSN: 0022-3263

DT

LΑ English

IT

77071-06-8P

RL: SPN (Synthetic preparation); PREP (Preparation) 77071-06-8 CAPLUS

RN

Benzamide, 4-bromo-N-(4,6-diamino-5-pyrimidinyl)- (9CI) (CA INDEX NAME) CN

GI

$$N = NNH$$

$$N =$$

Adenine, adenosine and 5'-adenylic acid react readily with benzenediazonium ion and its derivs. at pH 8-11 to yield derivs. of (E)-6-(3-phenyl-2-triazen-1-yl)purine, e.g., I (R = H, Me, Br, SO3H). triazenes decomp. in basic aq. soln. at 60-90.degree. to produce 8-aryladenines, apparently via intermol. processes. For adenosine and 5'-adenylic acid, the ribose residues are cleaved during this process. Both p-RC6H4N2+ and p-RC6H4.bul. can be intercepted during the reaction. Consequently, the phenylation reaction may be confidently formulated as an

L3 ANSWER 62 OF 147. CAPLUS COPYRIGHT 2003 ACS on STN AN 1994:645130 CAPLUS 1001. DN 121:245130 TI Selective Inhibition of Trypanosomal Glyceraldehyde-3-phosphate Dehydrogenase by Protein Structure-Based Design: Toward New Drugs for the Treatment of Sleeping Sickness Verlinde, Christophe L. M. J.; Callens, Mia; Van Calenbergh, Serge; Van ΑU ...3 Aerschot, Arthur; Herdewijn, Piet; Hannaert, Veronique; Michels, Paul A. Pasell M.; Opperdoes, Fred R.; Hol, Wim G. J. IMSchool of Medicine, University of Washington, Seattle, WA, 98195, USA Journal of Medicinal Chemistry (1994), 37(21), 3605-13 C\$ . DN CODEN: JMCMAR; ISSN: 0022-2623 DT Journal LA English ΑJ TI '73340-78-0P, 8-Phenyladenosine 158555-06-7P 1:5 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study; unclassified); PRP (Properties); SPN (Synthetic preparation); THU 30 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (protein structure-based design of selective inhibition of glyceraldehyde phosphate dehydrogenase complexes of humans and Trypanosoma brucei in treatment of sleeping sickness) RN 73340-78-0 CAPLUS Adenosine, 8-phenyl- (9CI) (CA INDEX NAME) CN Absolute stereochemistry.

RN 158555-06-7 CAPLUS CN Adenosine, 8-(2-thienyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Within the framework of a project aimed at rational design of drugs against diseases caused by trypanosomes and related hemoflagellate parasites, selective inhibitors of trypanosomal glycolysis were designed, synthesized, and tested. The design was based upon the crystallog. detd. structures of the NAD:glyceraldehyde-3-phosphate dehydrogenase complexes of humans and Trypanosoma brucei, the causative agent of sleeping sickness. After one design cycle, using the adenosine part of the NAD cofactor as a lead, the following encouraging results were obtained: (1) a 2-Me substitution, targeted at a small pocket near Val 36, improves inhibition of the parasite enzyme 12.5-fold; (2) an 8-(thien-2-yl) substitution, aimed at Leu 112 of the parasite enzyme, where the equiv. residue in the mammalian enzyme is Val 100, results in a 167-fold better inhibition of the trypanosomal enzyme, while the inhibition of the human enzyme is improved only 13-fold; (3) exploitation of a "selectivity cleft" created by a unique backbone conformation in the trypanosomal enzyme near the adenosine ribose yields a considerable improvement in selectivity: 2'-deoxy-2'-(3-methoxybenzamido)adenosine e inhibits the human enzyme only marginally but enhances inhibition of the parasite enzyme 45-fold when The designed inhibitors are not only better